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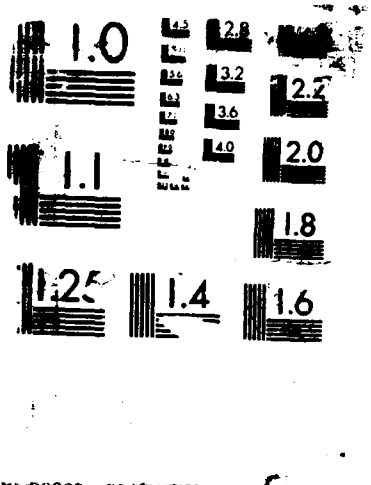

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19. ABSTRACT (Continue on reverse if necessary and identify by block number)

During the period covered by this report, six plenary meetings of the Chemistry Research-evaluation Panel for the Air Force Office of Scientific Research have been held: at Santa Fe, New Mexico on November 8 and 9, 1984; at Baltimore, Maryland on May 9 and 10, 1985; at Galveston, Texas on November 14 and 15, 1985; at Alexandria, Virginia on May 15 and 16, 1986; at the US Air Force Academy, Colorado on November 13 and 14, 1986; and at Georgetown University on May 14 and 15, 1987. During the period of this report, a total of two hundred and ninety-four proposals in the chemical and atmospheric sciences were evaluated and ranked. Panels of evaluators were provided for contractors' meetings that dealt with specific portions of the on-going Air Force Office of Scientific Research chemistry research program. These meetings were held in Albuquerque, New Mexico in October, 1984; in Dayton, Ohio in November, 1985 and in Bedford, Massachusetts in October, 1986. Reports covering each of these meetings have been submitted.

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22c. OFFICE SYMBOL NC	

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Georgetown University
Department of Chemistry

Final Technical Report
Contract F49620-84-C-0073

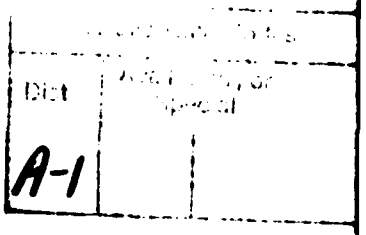
U.S. Air Force Office of Scientific Research
For the period September 10, 1984 to September 14, 1987

An earlier comprehensive interim technical report was submitted to cover the period from September 10,1984 to June 5, 1986.

During the period covered by this report, six plenary meetings of the Chemistry Research-evaluation Panel for the Air Force Office of Scientific Research have been held. The sixty-ninth chemistry research evaluation meeting for Air Force Office of Scientific Research was held at Santa Fe, New Mexico on November 8 and 9, 1984; forty proposals were considered at that meeting, and relative rankings for scientific quality were determined. An interim technical report specifying that rank-order (including atmospheric-science proposals) has been submitted and is appended as Appendix I. The seventieth chemistry research-evaluation meeting for the Air Force Office of Scientific Research was held at Baltimore, Maryland on May 9 and 10, 1985; sixty-one proposals were considered at that meeting, and relative rankings for scientific quality were determined. An interim technical report specifying that rank-order (including atmospheric-science proposals) has been submitted and is appended as Appendix II. The seventy-first chemistry research-evaluation meeting for the Air Force Office of Scientific Research was held at Galveston, Texas on November 14 and 15, 1985; sixty-three proposals were considered at that meeting, and relative rankings for scientific quality were determined. An interim technical report specifying that rank-order (including atmospheric-science proposals) has been submitted and is appended as Appendix III. The seventy-second chemistry research-evaluation meeting for the Air Force Office of

Scientific Research was held at Alexandria, Virginia on May 15 and 16, 1986; fifty-eight proposals were considered at that meeting, and relative rankings for scientific quality were determined. An interim technical report specifying that rank-order (including atmospheric-science proposals) has been submitted and is appended as Appendix IV. The seventy-third research-evaluation meeting was held at The U.S. Air Force Academy, Colorado on November 13 and 14, 1986; thirty-three proposals were considered at that meeting, and relative rankings for scientific quality were determined. An interim technical report specifying that rank-order (including atmospheric-science proposals) has been submitted and is appended as Appendix V. The seventy-fourth chemistry research-evaluation meeting was held at Georgetown University on May 14 and 15, 1987; thirty-nine proposals were considered at that meeting, and relative rankings for scientific quality were determined. An interim technical report has been submitted and is appended as Appendix VI. During the period of this report, a total of two hundred and ninety-four proposals in the chemical and atmospheric sciences were evaluated and ranked.

Panels of evaluators were provided for contractors' meetings that dealt with specific portions of the on-going Air Force Office of Scientific Research chemistry research program. These meetings were held in Albuquerque, New Mexico in October, 1984; in Dayton, Ohio in November, 1985 and in Bedford, Massachusetts in October, 1986. Reports covering each of these meetings have been submitted.



Persons who have served as members of Chemistry and atmospheric-science evaluation panels during this period include:

Professor Claude F. Bernasconi
Department of Chemistry
The University of California
Santa Cruz, California 95064

Dr. Enrico Clementi
IBM Fellow
IBM Corporation,
Kingston, New York 12401

Professor Joyce Y. Corey
Department of Chemistry
The University of Utah
Salt Lake City, Utah 84112

Dr. Joseph E. Demuth
Thomas J. Watson Research Center
IBM Corporation
Yorktown Heights, New York 10598

Dr. Jimmie D. Doll
Department of Chemistry
Los Alamos National Laboratory
Los Alamos, New Mexico 87545

Professor Dennis H. Evans
Department of Chemistry
The University of Wisconsin
Madison, Wisconsin 53706

Dr. George S. Hammond
Director
Integrated Chemical Systems
Laboratory
Allied-Signal Corporation
Morristown, New Jersey 07960

Professor William B. Hanson
Director
Center for Space Sciences
The University of Texas, Dallas
Richardson, Texas 75080

Professor H. James Harwood
Chairman
Institute of Polymer Science
University of Akron
Akron, Ohio 44325

Professor James Holton
Department of Atmospheric Science
The University of Washington
Seattle, Washington 98195

J. J. Lagowski
Piper Professor of Chemistry
The University of Texas
Austin, Texas 78712

Professor Donald Levy
Chairman, Department of Chemistry
The University of Chicago
Chicago, Illinois 60637

Professor Robert J. Madix
Department of Chemical Engineering
Stanford University
Stanford, California 93405

Professor C. Bradley Moore
Chairman, Department of Chemistry
The University of California
Berkeley, California 94720

Professor Royce W. Murray
Department of Chemistry
The University of North Carolina
Chapel Hill, North Carolina 27514

Professor Robert Silbey
Department of Chemistry
Massachusetts Institute of Technology
Cambridge, Massachusetts 02139

Professor William C. Stwalley
Department of Chemistry
The University of Iowa
Iowa City, Iowa 52242

Professor Richard P. Van Duyne
Department of Chemistry
Northwestern University
Evanston, Illinois 60201

Dr. Field H. Winslow
Bell Laboratories
600 Mountain Avenue
Murray Hill, New Jersey 07974

Teams of evaluators were provided on several occasions to evaluate portions of the research program of the Air Force Office of Scientific Research. Teams evaluated contractors' meetings in the field of chemical dynamics held in the Fall of each of the three years covered by the contract; in October, 1984 in Albuquerque, New Mexico, in November, 1985 in Dayton, Ohio and in November, 1986 in Concord, Massachusetts. Interim technical reports have been submitted to cover these activities.

A special research-evaluation panel was constituted for the purpose of advising the Director of Chemical Sciences, Air Force Office of Scientific Research, and other appropriate Air Force officers and civilian scientific officers concerning a program in high-energy-density materials being conducted by the Air Force Rocket Propulsion Laboratory. Two meetings were organized at which contractors and prospective contractors presented discussions of their scientific work, one in Washington, DC, March 20-21, 1986 and on in Rossyln, Va. on May 12 and 13, 1987. In connection with each of these contractor's meetings, and also in Lancaster, California on May 17 and 28, 1986 and at The U.S. Air Force Academy, Colorado on November 12 and 13, 1986 meetings of the high-energy-density-materials research-eveluation panel were held to consider proposals and to provide other evaluation of the high-energy-density program. A total of fifty-seven proposals was considered at these three meetings, and relative rankings for scientific quality were determined. Reports were submitted to cover these activities. An evaluation team was constituted to evaluate certain research being carried out at the California Institute of Technology. A report of findings of that evaluation was submitted. (Appendix VII)

Persons who have been members of the high-energy-density materials panel are:

Professor Charles F. Bender
Advanced Computational Methods Center
The University of Georgia
Athens, Georgia 30602

Professor William Happer
Department of Physics
Princeton University
Princeton, New Jersey 08544

Professor M. Frederick Hawthorne
Department of Chemistry
The University of California
Los Angeles, California 90024

Dr. Ronald R. Herm
The Aerospace Corporation
Los Angeles, California 90009

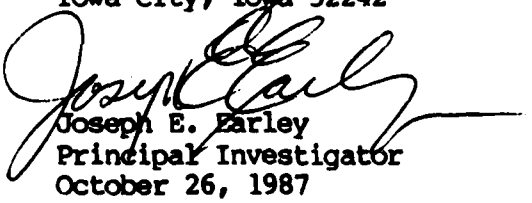
Dr. Marilyn E. Jacox
Molecular Spectroscopy Division
The National Bureau of Standards
Gaithersburg, Maryland 20899

Lewis H. Nosanow
Vice Chancellor for Research
The University of California
Irvine, California 92717

Professor Isaac F. Silvera
Lyman Laboratory of Physics
Harvard University
Cambridge, Massachusetts 02138

Professor William C. Stwalley
Iowa Laser Facility
The University of Iowa
Iowa City, Iowa 52242

Submitted by,



Joseph E. Earley
Principal Investigator
October 26, 1987

Georgetown University

Department of Chemistry

Revised Technical Report for AFOSR Chemistry Research-Evaluation

	Category I		Category II	
A	82	West	97	Crosley
			96	Bernasek
A-	80	Ault	64	Cowin
	79	Dovichi	70	Metiu
	78	DeLevie*	71	Redner
			74	Heaven
			65	Cool
			60	Miller
A-/B+			69	Thompson
			67	Gardner
B+	66	Weber	68	Wolf
	81	Horn	63	Liu/Ziv/Tsong
	86	Calcote	62	Rosenfeld
	93	Dresselhaus	73	Kaufman
	58	Bumgardner	95	Becker/Gillen
	89	Soong	75	Andermann
	76	Tilley		
	85	White		
B/B+	91	Blumstein		
B	84	Hosmane		
	94	Niemczyk		
	90	Chien		
	92	Tomozawa		
	87	Akinc		
	77	Shellhamer		

Ranking deferred:

78	DeLevie	98	Mukamel**
88	White/Kyu**		

* not ranked in conjunction with other A's
** additional review required

Joseph E. Earley
Professor and Chairman
Principal Investigator
December 5, 1984

Appendix II

Georgetown University

Department of Chemistry

Contract F49670-84-C-0073

Interim Technical Report for AFOSR Chemistry Research-Evaluation

	Category I		Category II	
A+			A+	15 Zare
				58 Wittig
A	50	Collman	A	30 Leone
	23	Tyler		07 Steinfeld
				32 Houston
				03 Pratt
				60 Benziger
				20 Crim
				47 Rossi
				37 Campion
				04 Kinsey
A-	11	Clearfield	A-	27 Bowers
	39	Dewar		02 Parmenter
	26	Nocera		24 George
	51	Reiss		56 Cooper
	46	Green		25 Dyke
	22	Clearfield		01 Sullivan
				41 Pimental
				55 Rothe / Reck
B+	42	Mamantov	B+	14 Raff
	57	Hughes		54 Topp*
	43	Trogler		53 Sloan
	40	Ewig / Van Wazer		12 Murray
	10	Koenig		31 Schwerzel*
	09	Weeks		28 Kupperman
	45	Klein		
	44	Smith		
B	08	Czarnik	B	52 Van Hove*
	34	Stimming		29 Lauer
	05	Cotts		
	06	Potember		
C	61	Bockris	C	13 Daily
	19	Toy		
	21	Levy		

*additional review suggested

Joseph E. Earley
Professor and Chairman
Principal Investigator
May 15, 1985

Appendix III

Georgetown University
Department of Chemistry

Interim Technical Report for AFOSR Chemistry Research-Evaluation

	Category I		Category II		Category III	
A	103	Stone	83	Yates	62	Tsunoda
	104	McCreery	76	Yarkony	73	Wickwar
			77	Goddard	71	McClure
A-	109	Ratner	92	Hemminger	64	Markson
	90	Geoffroy	89	Leventhal	69	Imhof
	91	Davis	75	McKoy	63	Dunkerton
	111	Anson	78	Engel		
	117	Gillis(*)	114	Martin		
	94	Lemal	88	Erskine		
			101	Nesbitt		
			124	Weisshar		
			120	Futrell		
			116	Bernstein		
			85	Golde		
			86	Slanger		
			70	Weltner		
			97	Adams		
B+	102	Brajter-Toth	107	Tolk	79	Bryson
	108	Weaver	121	Morse		
	93	Bennett	100	Trenary		
	115	Bunding	123	Vasudev		
	72	Welch	82	Ogilby		
	80	Caruso	67	Davis (rtn)		
	106	Isayev*	89	Davis (therm)		
			125	Glyde*		
			99	Jones & Weatherford*		
			87	Hopster*		
			113	Redner*		
B	98	Tien	96	Hudson	59	Lucas
			112	Andermann		
			118	Helvajian		
			119	Stedman		
			122	Denison		
			65	Ohrn and Zerner		
C	95	Kordas	81	McQuistan	66	Ganguly
	105	Brostow				
	110	Neelakantaswamy				

*tentative ranking, pending furthur rev

Joseph E. Earley
Professor and Chairman
Principal Investigator
November 18, 1985

Appendix IV

Georgetown University
Department of Chemistry

Interim Technical Report for AFOSR Chemistry Research-Evaluation
Contract F49620-84-C-0073

	Category I	Category II	Category III
A+		14 Zewail	
		18 Cavanagh	
A	51 Turro*	20 Heller	73 Wickwar
		25 Helm	74 Schotland
		13 Ross	128 Fritts
		51 Turro*	
		26 King	
		52 Schaefer	
A-	49 Eisenthal*	49 Eisenthal*	69 Imhof
	50 Weaver	05 Williams	127 Rahn
	43 McKinstry	08 Truhlar	129 Adams
	34 Martin	30 Weitz	27 Keyser
	39 Sneddon	44 Dyke	29 Liou
	35 Goldberg*	48 Marks	
		32 Madix*	
B+	21 Tomkiewicz	16 Schwartz	28 Warner
	40 Shreeve	24 Schulz	
	41 Wolczanski	15 Balasubramanian	
	02 Tidwell	23 Brumer	
	47 Berry	11 Streitwieser	
	37 Mauritz	36 Redmon	
	22 King	17 Stair	
	04 Ojima	09 Gordon	
	06 Nicholas	42 Sloan	
	32 Madix*	19 Adelman	
		45 Worsnop	
		35 Goldberg*	
		53 Somorjari	
		33 Graff	
B	01 Jones	46 Kupperman	
		12 Rice	
		10 Wulfman	
		38 Hamilton	
		03 Wachman	
		07 Avnir	
C	31 Deymier		130 Armstrong

Joseph E. Earley
Professor and Chairman
Principal Investigator
May 20, 1986

*in both I and II

Appendix V

Georgetown University
Department of Chemistry

Interim Technical Report for AFOSR Chemistry Research-Evaluation
Contract F49620-84-C-0073

	Category I	Category II	Category III	Category IV
A+				344 Moore 345 Lester
A	70 Ratner 82 Schrock	86 Neumark 80 Prasad*	60 Hernandez	314 Cassasa 320 Engelking 342 Bae 305 Carpenter
A-	65 Doherty 71 Ellis 80 Prasad*	55 Mukamel 73 Williams 56 Fano 77 Kolb 81 Guberman		302 Bernath 341 Daley 338 Schaeffer 340 Scobilgen 325 Weitz 319 Apkarian
B+	64 Holmes 83 Hosmane 74 Damrauer 72 Lagow 59 Norman 78 Wolfe	79 Rabitz# 54 Bauer 75 Leventhal 66 Page 88 Coombe 84 Fenn	68 Balachandran	311 Gilbert 315 Brener 333 Dagligian 335 Kirby 336 Hardwick 306 Politzer 334 Miller
B	58 White	76 Abeles 61 Peterson	69 D'Angelo 67 Pielke	343 Nicolaides 303 Eisenthal 331 Yarkony 309 Wight 301 Shearer 313 Allen 304 Nichol
C	63 Abrahamson	57 Khait 62 Brown		307 Davis 308 Ortiz 316 Garrett 323 McFarlane 346 Bass 347 Kumar
R				312 Haloulak

Joseph E. Earley
Professor and Chairman
Principal Investigator

November 14, 1986

*in both category I and category II
#additional reviews pending

Georgetown University
Department of Chemistry

Appendix VI

Interim Technical Report for AFOSR Chemistry Research-Evaluation

	Category I	Category II	Category III	Category IV
A	13 McCreery	33 Field 10 Leone 04 Smith 27 Hepburn	35 Cotton*	203 Grant 209 Kinkead (O_2-F_2 part)
A-	23 Verkade 09 Heinekan/Elder	28 Trenary 12 Winograd 26 Cooper 11 Eyler 17 Bernath 03 Marx 20 Kellmann		201 Politzer 206 Berkson
B+	31 Kuivila 19 King 29 Boudjouk 37 Fratini 08 Goodenough	16 Gole 15 Bauer 39 Oldenburg	06 Adams 36 Lee* 38 Uthe*	207 Dagdigian 204 Steadman 212 Hehre 202 Kirby
B	01 Huppert 14 Lee 34 Donahue 25 Welsh	07 Czanderna 24 Whitehead 21 Felder 22 Turner		205 Hardwick 213 Eisenthal 214 Harbottle* 208 Ortiz 209 Kinkead (Matrix part) 210 Allen
C	18 Mark	30 Bates# 32 Lowdin		211 Vernecker

Joseph E. Earley
Professor and Chairman
Principal Investigator

May 15, 1987

*tentative rating, pending further review.

#proposal insufficient and incomplete

DEPARTMENT OF THE AIR FORCE
AIR FORCE ASTRONAUTICS LABORATORY (AFSC)
EDWARDS AIR FORCE BASE, CALIFORNIA 93523-5000

RTAO: CX (Lt Lauderdale, 5413) 16 JUL 1987

SUBJ: Trip Report for Visit to the California Institute of Technology (Cal Tech) on 14 Jul 87

TO: CX
CC/CV/CA
IN TURN

1. Abstract. On 14 Jul 87, Lt Walter Lauderdale visited Prof Aron Kuppermann at the California Institute of Technology. Accompanying him on this visit were Dr William Stwalley and Dr Ron Herm, chairman and member of the High Energy Density Matter (HEDM) technical evaluation panel, respectively. The purpose of this visit was to evaluate the technical progress and future plans of contract F04611-86-K-0076, "Experimental Studies of the Properties of Trihydrogen and Tetrahydrogen". The evaluation was prompted by three factors: 1) the seeming lack of progress in the project, 2) the high cost of the overall contract, and 3) FY88 budget constraints.

2. Background. On the morning of 14 Jul 87, prior to the meeting with Prof Kuppermann, Lt Lauderdale met with Dr Herm and Dr Stwalley to discuss the history of Prof Kuppermann's work for the AFAL. Copies of all progress reports and the technical portion of the original proposals, along with the program plans were sent to them earlier. Prof Kuppermann's first contract to the AFAL was awarded in response to the original tetrahydrogen PRDA. This project set ambitious goals of performing H_3^* + HI crossed beam experiments to determine the possible existence of H_4. During the course of the project, numerous setbacks occurred due to a large attenuation of the H_3 beam intensity when the source was mated to the crossed beam chamber. The final result of the original contract was a redesigned H_3 source and increased awareness of unforeseen difficulties, but no conclusive crossed beam experiments were performed (see AFRPL-TR-86-103, attached). The current contract is a continuation of this effort. During the first 11 months of the present effort, problems with H_3 beam intensity have continued to plague the research. Improvements have been made incrementally and systematically over this time and have resulted in a methodology to locate and center the H_3 beam. This provides the intensity, but it is still 3 orders of magnitude less than in the original H_3 beam apparatus. The progress to date of the current contract is summarized in the attached quarterly report. This report was submitted as a precursor to the on-site evaluation. Dr Herm and Dr Stwalley were asked to assist in the evaluation in view of their respective backgrounds in molecular beams and in their role as members of the HEDM technical evaluation panel.

3. Results. Prof Kuppermann revieved his work and was asked questions by Dr Herm and Dr Stvalley during this time. A summary of this discussion is detailed follows.

a. The H3 beam source is initially aligned optically. However, when the arc discharge is started, the H3 beam does not follow the optical axis. Therefore, the beam never appears at the detector because it never passes through the slit aperture downstream. The beam was found by using a larger slit, but a larger slit leads to poor collimation of the beam and a low intensity in the crossed beam interaction region. The solution has been to use a diaphragm slit which can be opened wide (12 mm) to allow location of the beam. The entire source and support structure is then physically rotated around an axis which passes through the arc discharge port. This then brings the beam into the center of the diaphragm and the diaphragm is then closed down to the operating diameter (2 mm).

b. This final solution has consumed the better part of two years (over both contracts). The reasons for this has been that Prof Kuppermann is developing a technology that is available nowhere else. While H3 has been made and characterized by several groups, no other group has a source of any metastable which is as intense as Kuppermann's (in the original H3 beam configuration). Many different variables have had a drastic affect on beam intensity and alignment. These include, but it not limited to, the pressure of the H3 arc source cooling water, the grade of titanium metal used for the anode and cathode of the arc discharge, and the intensity of the background light emitted from the arc discharge (reflected in the current solutions to avoid the light problem within the detector). The affect of these variables, for the most part, were unforeseeable. Also, since this is a unique arc source, the problems could only be discovered after many runs and an examination of the empirical evidence. These were in addition to the normal operating parameters of the experiment such as slit width, skimmer distance, H2 back pressure, discharge voltage, downstream pressure, and all aperture widths, to name a few.

c. The collimation requirement for the beam is quite stringent. This is because the angular region of interest for the scattering experiments is within several degrees of the peak in the H3 beam intensity. If the beam is not well collimated, then its signal will mask the signal from the scattered products of the crossed beams. Closing the aperture to achieve good collimation, however, is useless if the beam does not pass through the resulting slit. This demonstrates how crucial the alignment is in this experiment. In addition, there are still some questions that should be answered about the H3 beam source itself. All of the issues are to be addressed in the H3 phase of the contract, which is scheduled to start upon completion of the H4 work.

4. Conclusions. Taking into consideration all the results and the discussions with Dr Herm and Dr Stvalley, conclusions are:

a. The H3 beam source still requires characterization and refinement independent of the H4 experiment.

b. In retrospect, the HEDM panel and the AFAL made a mistake in having Prof Kuppermann do the H4 work before the H3 work, which is reversed from the proposal. Prof Kuppermann made a mistake in agreeing to the change. Many of the problems he has run into may have been solved in the H3 work. Doing the H4 work first, however, made sense at the initiation of the contract because H4 was a highly visible part of the ARIES program.

c. The current crossed beam chamber is antiquated. Its use forces a long H3 beam path and attenuates the intensity greatly (intensity is proportional to $1/r^2$). Also, other detection methods which are more sensitive are too large to fit within the chamber, also affecting intensity measurements.

d. Given the current laboratory apparatus, Dr Stvalley and Dr Herm felt that Prof Kuppermann's approach to the problems has been acceptable.

e. Dr Herm and Dr Stvalley believe that conclusive crossed beam results will not occur for at least six months. They also feel that the H4 work should be given no more than 12 months more effort.

f. Dr Herm and Dr Stvalley both emphasize that Prof Kuppermann's work is at a level more basic than fundamental research. The technology of the intense metastable H3 beam is important scientifically. By the very nature of its development, it is difficult to predict all the problems to be surmounted.

g. Dr Herm and Dr Stvalley believe that a well characterized H3* source is a very valuable asset to the ARIES program's search for new, novel energetic species. H3* is a very energetic reactant which could be combined with other species to yield a new, high energy density molecule.

5. Recommendations. The recommendations for actions regarding this contract are:

a. Give approval for Prof Kuppermann to begin the work on H3.

b. Pass along suggestions from Dr Herm and Dr Stvalley on Prof Kuppermann's experimental procedures.

c. Negotiate a modification to the contract to suspend the H4 work and place an option to continue it after the H3 work has been completed. The decision to continue the H4 work will be based on the H3 work and the H4 work (theoretical and experimental) being done by other HEDM contractors.

d. Negotiate to delete the purchase of an additional quadrupole mass spectrometer for the H3 work (Dr Herm and Dr Stvalley feel the mass spectrometer used in the original H3 work will be sufficient for

the proposed B3 work).

e. Discuss the possibility of stretching out the effort to ease the budgetary pressure in FY88.

f. Adjust the HEDM FY88 budget (Cluster D-7) to reflect continuation of this contract.

WALTER J. LAUDERDALE, 1Lt, USAF
Project Manager

2 Atch
1. AFRPL-TR-86-103
2. Progress Report

END
DATE
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